Effective Potentials: A New Approach and New Results for One-Dimensional Systems with Competing Length Scales

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A new method, involving the solution of a nonlinear eigenvalue equation, is proposed for finding the ground-state configurations and energies of the Frenkel-Kontorova and similar one-dimensional models which can show complicated transitions between commensurate and incommensurate phases. It is used to show that a distinctive phase diagram can arise if a cosine potential is perturbed by the addition of suitable harmonics.

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Commensurate-incommensurate phase transitions pose a number of interesting and challenging theoretical problems.[1] One difficulty in studying them is the scarcity of exactly solvable models. Even one-dimensional, classical systems with nearest-neighbor interaction at zero temperature and competing length scales turn out to have a wealth of interesting properties which are still not very well understood. (There is an enormous literature on the subject; we refer the reader to some of the more recent works.[2-11]) This paper describes a method for studying such one-dimensional systems by use of a functional equation for an "effective potential," (8) below, and presents a new type of phase diagram obtained by this means.

Consider a one-dimensional system of atoms with a potential energy

$$H(\{u_n\}) = \sum_n [W(u_{n+1} - u_n) + V(u_n)], \quad (1)$$

where u_n is the position of the nth atom, W is the potential energy of a spring connecting two neighboring atoms a distance y apart, and

$$V(u+1) = V(u) \quad (2)$$

is a periodic potential. The particular case

$$W(y) = \tfrac{1}{2}(y-\gamma)^2, \quad (3)$$

$$V(u) = K(1-\cos 2\pi u)/(2\pi)^2, \quad (4)$$

is often called the Frenkel-Kontorova[12] model. The problem is to find the ground-state energy per particle λ and the configuration of atoms in the ground state(s) as a function of parameters such as γ and K. When $K=0$ the atoms will be regularly spaced with separation γ, whereas when K is sufficiently large they will (unless γ is half an odd integer) all be at minima of the potential. Thus there are two competing length scales, and at intermediate values of K a very complex behavior can occur, with either commensurate phases in which u_n modulo 1 is a periodic function of n, or incommensurate phases.

A number of studies[8-11] of the ground states of (1) have been based upon searches for solutions to the equilibrium equations

$$\partial H/\partial u_n = 0. \quad (5)$$

In particular, it is possible to relate u_{n+1} to u_n and u_{n-1} through an area-preserving two-dimensional map, which can then be studied numerically or by methods applied to other dynamical systems.[13-16] Not surprisingly, the mapping problem turns out to be just as challenging as the original ground-state problem, or even more so since not only the ground state but also various metastable and unstable configurations satisfy (6).

Our approach, by contrast, consists of looking for configurations of atoms in which (1) is actually a minimum in an appropriate sense, and thus resembles some work of Aubry.[2,3] It is based on the following physical picture. Suppose that an atom moving in an arbitrary periodic potential

$$U(u+1) = U(u) \quad (6)$$

is connected by a spring to a second atom moving in the periodic potential V; see Fig. 1. For a fixed position u' of the second atom, the minimum energy of the combined system is

$$\bar{U}(u') = \mathscr{K} U(u') = V(u') + \min_u [W(u'-u) + U(u)], \quad (7)$$

where the expression in the second line defines the nonlinear functional transformation $\mathscr{K}$. In particular, when $U=V$, $\mathscr{K}V(u')$ is the minimum energy of two atoms in the common potential V connected by a spring, provided that one of them is fixed at u'. Simi-

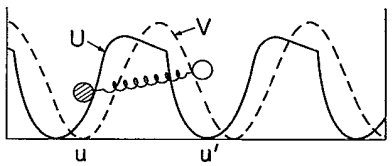

FIG. 1. The potentials $U(u)$ and $V(u')$.

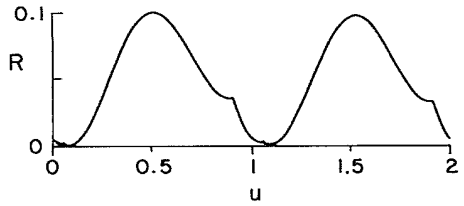

FIG. 2. The effective potential $R(u)$ for $K=3$, $\gamma=0.36$.

larly, if the functional transformation is iterated n times, $\mathscr{K}^n V$ is the minimum energy of a chain of n atoms in the potential V, provided that the right-most atom is at a specified position. Note that $\mathscr{K}^n V$ has the same periodicity as V. Thus as n tends to infinity it is plausible that V and $\mathscr{K}^n V$ will differ by $n\lambda$ plus some oscillatory term of order 1. Rather than looking at iterates of $\mathscr{K}$ it is convenient to search for a periodic $[R(u)=R(1+u)]$ solution to the nonlinear "eigenvalue" equation

$$\mathscr{K}R(u')=\lambda+R(u')$$
$$=V(u')+\min_u[W(u'-u)+R(u)]. \quad (8)$$

Provided that V is continuous and periodic *à la* Eq. (2), and W is continuous and bounded below, one can show that (8) always possesses a continuous periodic solution R, and the corresponding λ is unique (for given V and W). In addition, the (in general one-to-many) map

$$u=\tau(u') \quad (9)$$

obtained by noting which u minimizes the right-hand side of (8) can be employed to generate a ground-state configuration of atoms $\{u_n\}$. (More details will be given in a later publication.) Another procedure for obtaining Eq. (8) is to consider a transfer matrix and take the limit as the temperature goes to zero.[17]

A straightforward numerical approach to the study of (8) is to impose a grid of a hundred (or more or less) equally spaced points in the unit interval and then apply $\mathscr{K}$ to functions defined on these points. A solution to (8) can be obtained by insertion of a first approximation on the right-hand side to generate a function which when averaged with the first gives the second approximation, and so forth. The corresponding map (9) can then be iterated to find a ground-state configuration.

As an example, Fig. 2 shows R for $K=3$ and $\gamma=0.36$, under the assumptions (3) and (4), while Fig. 3 shows the corresponding function τ. Note that R is continuous but has a discontinuous first derivative at the same points where τ is discontinuous. This is what one expects in a situation in which the ground state is "pinned" to the periodic potential, whereas one expects R and τ to be smooth functions when the chain of atoms can "slide" under zero force.[2,9]

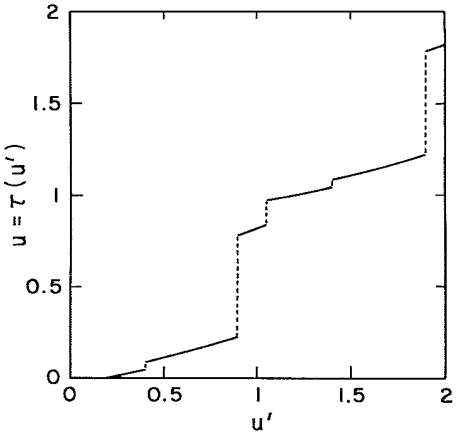

FIG. 3. The mapping $u=\tau(u')$ corresponding to Fig. 2.

A portion of the phase diagram[18] in the (γ,K) plane is shown in Fig. 4. One expects an infinite number of "tongues" corresponding to commensurate phases with different rational values of the winding number ω (average separation between neighboring atoms), in analogy with Aubry's results for a potential V of repeating parabolas.[19]

However, a very different type of phase diagram is possible, as shown in Fig. 5, with a potential

$$V(u)=\frac{K}{(2\pi)^2}[1+\epsilon-\cos 2\pi u-\epsilon\cos 4\pi u], \quad (10)$$

with $\epsilon=0.1$. Note that the tongues are now split by horizontal lines at which there is a "first-order" transition between distinct ground states having the same winding number. The phases marked A are similar to those which arise with use of (4), whereas in those marked B there is an atom located at $u=\frac{1}{2}$, the maximum of the potential. Our numerical studies, which use the more conventional approach based on (5) in addition to (8) in order to locate the transition points precisely, strongly suggest that the number of such horizontal bars increases with increasing Q for a rational winding number $\omega=P/Q$. There are special

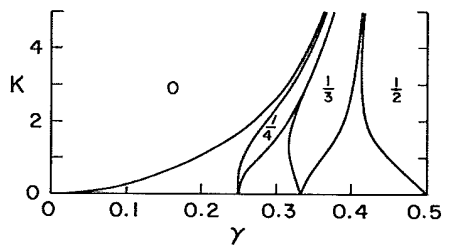

FIG. 4. Phase diagram for the Frenkel-Kontorova model. The numbers are values of the winding number ω. The unlabeled regions contain additional structure, as in Fig. 25 of Ref. 1.

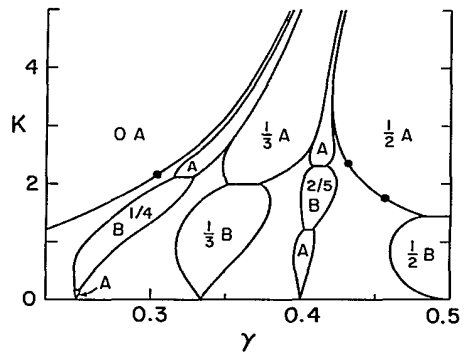

FIG. 5. Phase diagram for V given by Eq. (10) with $\epsilon=0.1$. The solid circles are some of the points on the boundaries of $\omega=0$ and $\omega=\frac{1}{2}$ where horizontal bars accumulate.

points on the boundaries of phases with rational ω which are apparently points of accumulation of these bars, and where the boundary has a discontinuous slope. Figure 5 shows one such point on the boundary of $\omega=0$ and two on the boundary of $\omega=\frac{1}{2}$. At these values of K the minimum-energy soliton ("kink" or "discommensuration") changes its character. It seems likely that there are infinitely many such accumulation points, and hence accumulation points of these accumulation points.

The behavior shown in Fig. 5 does not depend on the precise choice of ϵ, but seems to be present for a range of ϵ values beginning at (but not including) $\epsilon=0$, whereas for $\epsilon\leq 0$ we find diagrams topologically similar to Fig. 4. Instead of a second harmonic, one can add a third harmonic [replace 4π in (10) by 6π] and obtain a diagram similar to Fig. 5, with in this case $\epsilon<0$. Thus the simple cosine (4) appears to be on the borderline between two very different types of behavior.

One advantage of (8) over alternative approaches to the study of this class of problems is that *there is no need that W in (1) be a convex function.* Both the approach of Aubry[2,3] and those[8-11] based directly on the mapping associated with (6) make use of the convexity of W in an important way. They are thus not immediately applicable to a case such as

$$W(y)=1-\cos 2\pi(y-\gamma), \tag{11}$$

which when combined with (4) is equivalent to a one-dimensional classical xy model with a chiral interaction placed in an external magnetic field (proportional to K). We find that a numerical study based on the minimization equation (8) works just as well with (11) as (3) and yields a phase diagram which is significantly different from cases in which W is convex. Details will be reported in a later publication.

Whether or not W is convex, solving (8) yields the ground state rather than a metastable or unstable state. The main disadvantage in using (8) is that one must solve for a function R which contains much more information than is present in the ground state. This additional information is sometimes useful; for example, in calculating the energies of the solitons which determine the range of γ values over which some ω is stable.[20]

In summary, the functional equation (8) provides a new tool for studying the ground states of systems of the type (1), and the phase diagram in Fig. 5 illustrates its utility.

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